

## Article

# Atomistic Study of the Interaction Nature of H-Dislocation and the Validity of Elasticity in Bcc Iron

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**Abstract:** One way to assess the validity of elasticity is with the method of atomic simulations. Molecular statics (MS) simulations are performed to study the interactions between H and edge dislocations in bcc iron using embedded-atom-method potential for a Fe-H system. The nature of H-dislocation interactions can be investigated and the validity of elasticity can be examined. We show that the sites with strong binding energy are found at the dislocation core, as well as in the slip plane, suggesting high H concentrations can form along the slip plane. It is found that the interstitial H not only interacts with hydrostatic stress, but also with the shear stresses generated by the dislocation, especially on the slip plane. When the dislocation stresses are represented using anisotropic elasticity, the validity of elasticity is at H-dislocation distance larger than  $\sim 19$  Å, i.e., the same as the isotropic predictions. When H lies closer to the dislocation, good agreement with simulations is obtained if considering all strains induced by H at the octahedral sites and using anisotropic elasticity.

**Keywords:** edge dislocation; elastic theory; hydrogen; binding energy; slip plane



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## 1. Introduction

Hydrogen embrittlement (HE) has been a long-standing, unresolved problem for the safe use of almost all materials. Extensive researches have clarified that one of the predominant reasons for HE is the interaction between H and dislocations [1–3]. In situ straining in an environmental cell transmission electron microscope (TEM) showed that H increases the mobilities of dislocations. Microscopic observations in austenitic stainless steels, Al, Ni-Co and Ni revealed that H can inhibit cross-slip of dislocations, inducing slip planarity [4,5]. The microstructure of fracture samples examined by TEM provided evidence that H-induced flat fracture surfaces are the results of the activities of intensive dislocations immediately beneath them. In situ electrochemical nanoindentation (ECNI) showed that H enhances homogeneous dislocation nucleation (HDN) [6–8].

The prerequisite for H affecting dislocation activities is H binding around or interacting with dislocations. The H-dislocation interactions can be modeled directly by atomistic simulations. For example, density function theory (DFT) calculations [9] and molecular static (MS) simulations [10,11] have given the binding energies of a single H atom with dislocations. More details of the interactions, including H binding sites [10], distribution of binding energies [12], and H migration path [10–13] have been discussed carefully. However, atomistic studies are mostly focused on the simple cases where H is interacting with only one or two dislocations, or H is binding around a slow dislocation [14–16]. When the interactions occur between H atoms and multiple dislocations and cost a lot of time (e.g., H diffusion to dislocations), atomistic simulations are not so applicable.

Alternatively, elasticity theory is also extensively used to study solute-dislocation interaction [17,18]. Cottrell et al. [19,20] gave the detailed theory of the distribution of solute atoms which interact weakly with a slowly gliding dislocation. They first modelled solute atoms as elastic inclusions in an isotropic continuum matrix and considered the strains induced by solutes were homogeneous; the binding energy was estimated as the elastic interaction between the pressure created by a dislocation and the volume change induced by solutes. This assumption may be valid for interactions between vacancies or substitutions with dislocation. However, for interstitials (such as C interstitial in bcc Fe), where the generated strains by interstitials are asymmetric, the above assumption may be questionable. To overcome this shortcoming, Cochardt et al. [21] improved Cottrell's work by taking the interaction between shear strain associated with solutes and shear stress created by a dislocation into consideration. Later, the dislocation stress field calculated using anisotropic elasticity was applied to describe solute-dislocation interaction [22]. Up to now, elasticity has been widely applied to investigate the solute atmosphere around dislocation, dislocation motion with solutes, solute-dislocation junction interaction, and solute strengthening of dislocation [14,23–25]. Despite its wide success, the reliability and accuracy of elastic theory remains to be examined.

One way to assess the validity of elasticity is with the method of atomic simulations (e.g., DFT, MD/MS). In this way, solute-dislocation interaction obtained from elasticity and simulations are compared, the valid range of elasticity can therefore be carried out and the proper refinement can be made [26,27]. Such an approach has been applied to study the interaction between interstitial Ni and edge dislocation in fcc Ni [28]. It showed that interaction energy calculated using isotropic elasticity yields reasonable agreement with atomistic results if the distance between the interstitial Ni atoms and the dislocation core is further than  $3b$  ( $\sim 7.5$  Å). Clouet et al. [29] investigated the applicability of isotropic elasticity and anisotropic elasticity to C-dislocation interactions in bcc iron and found that if considering both the dilatation and the tetragonal distortion induced by C, anisotropic predictions quantitatively agree with simulation results. Further, they discussed the valid range of anisotropic elasticity and found that, for a screw dislocation, C-dislocation binding energy predicted by anisotropic elasticity is in very good agreement with atomistic simulations except for the dislocation core; for an edge dislocation, the elasticity only models C-dislocation interactions at a distance greater than 20 Å from the core. For the lighter H atom, the validity of elastic predictions has been identified in fcc Ni [28,30]; however, in bcc iron, where H usually occupies a tetrahedral site and causes asymmetric strains, the reliability of elasticity has not been examined.

In this study, MS simulations are performed to study the interactions between H and edge dislocations in bcc iron using embedded-atom-method potential for the Fe-H system. Interactions computed by MS are then compared with elasticity theory. Therefore, the nature of H-dislocation interactions can be investigated and the validity of elasticity can be examined.

## 2. Atomistic Simulations

### 2.1. Interatomic Potential

For Fe-H system, a Finnis–Sinclair (F–S) type EAM potential, newly developed by Wen et al. [18], is applied to describe the interatomic behaviors. The Fe-Fe interaction of this potential is taken from the work of Ramasubramaniam et al. [10,11], which predicts the compact core structure of the screw dislocation in bcc iron based on density function theory (DFT) calculations. The cross Fe-H interaction and the H-H interaction of the potential is reproduced based on our DFT calculations, which describes repulsive H-H interactions. The binding energy distribution of H and dislocation was obtained by atomic simulation. According to the distribution of hydrogen binding energy near the edge dislocation, the maximum binding energy is 0.46 eV. Similarly, we also calculate the distribution of hydrogen binding energy near the screw dislocation. The maximum binding energy is 0.30 eV, which is close to the results of DFT calculations [31] and other

atomic simulations [9]. The location of the maximum binding energy is near the dislocation core  $\sim 3.0$  Å, while the attraction of hydrogen atoms to the geometrical center of the screw dislocation is weak. Due to the structural characteristics of the triple symmetry of the screw dislocation core, the geometric shape of the position of the maximum binding energy is triple-symmetric about the elastic center of the dislocation, which is consistent with the DFT results. Thus, this new potential can avoid unrealistic clustering of H atoms. The new EAM potential accurately reproduces the dissolution heat of H (0.33 eV) in bcc Fe, and the binding energies of H with edge (0.47 eV) and screw (0.30 eV) dislocations, which are in excellent agreement with DFT results.

## 2.2. Details of Atomistic Simulation

A cylindrical cell with a radius of 15 nm and a length of  $\sim 2$  nm along the  $z$  axis is created for simulations. An edge dislocation is placed at the center of the cylinder, with  $x$ ,  $y$ , and  $z$  axes parallel to  $[111]$ ,  $[-110]$  and  $[-1-12]$  directions. The dislocation is designed with linear direction along  $z$  axes and created by displacing the atoms according to their displacement fields calculated from the sextic formalism of Stroh. Periodic boundary conditions are applied in the  $z$  directions. Atoms located in the outer shell of the cylinder with a thickness of 1 nm are fixed, while the other atoms are allowed to move freely in the relaxation process. After the creation of an edge dislocation, the whole system is relaxed under the above boundary conditions by the conjugate gradient (CG) method.

## 3. Results

### 3.1. Atomistic Binding Energy

After relaxation of the dislocation, a H atom is introduced into the simulation cell to study H-dislocation interactions. Possible H-occupying sites in bcc iron are tetrahedral sites (T sites) and there are six T sites around a central Fe. Since there are four layers of Fe atoms packing along the  $[-1-12]$  directions, any one layer of them was chosen as the central atoms. All the T sites around these Fe atoms are considered as the H pre-placing sites. Then, the simulation cell containing H and the dislocation was relaxed using the CG method again.

The binding energy  $E^b$  between H and the dislocation is estimated as:

$$E^b = E^d + E^H - (E_d^H + E^0) \quad (1)$$

where  $E^d$  is the energy of the system containing the dislocation,  $E^H$  is the energy of the system containing one H atom at T site,  $E_d^H$  is the energy of the system containing one H atom and the dislocation, and  $E^0$  is the energy of the perfect lattice. By this estimation, a positive binding energy indicates attraction between H and the dislocation.

Following the above description, the binding energies of H around the dislocation can be obtained. It is found that if the initial separation distance between H and dislocation is less than 1 nm and there are only constraining atoms in the outer shell of the cylinder during relaxation, the dislocation can be attracted by H and slip toward it. The obtained binding energy is in fact the binding energy between H and dislocation core. A similar phenomenon is also observed in H-dislocation interactions in fcc Ni [32]. The explanation for this phenomenon is simply that the attractive force at short H-dislocation distance is larger than the Peierls stress ( $\sim 1$  MPa/Å) of the straight edge dislocation in Fe [33,34]. In order to obtain accurate H-dislocation binding energies, when relaxing, only Fe atoms in the neighborhood of the interstitial H are allowed to move, while other atoms are fixed to constrain the dislocation. Because H-induced distortion in bcc Fe occurs in short range and the content is very small, fixing atoms away from H may not influence H-dislocation interactions. It is found that fixing atoms 5 Å away from H is proper to describe H-dislocation interactions, since this produces the maximum binding energy of 0.468 eV, which is only 0.4% lower than the binding energy (0.47 eV).

### 3.2. Results of Atomistic Simulations

H binding energies are displayed as a function of H positions in Figure 1, where Fe atoms are represented as small black spheres, and H positions are represented as large spheres. Sites with strong H-dislocation binding energy are distributed around the dislocation core. The maximum H-dislocation binding energy arises just beneath the slip plane, at a distance of  $\sim 1.5$  Å from the core. The maximum binding energy is 0.468 eV. It is noted that the binding energy spreads widely in the slip plane in Figure 1. The similar observations are obtained in interactions between H and an  $\langle 111 \rangle$   $\{112\}$  edge dislocations, as well as between H and  $\{111\}$   $\langle 110 \rangle$  edge dislocation in Ni. It seems likely that H distribution can spread in the slip planes of edge dislocations whether the core structure is compact or dissociated [35]. This is contrary to the isotropic elasticity in that there is no interaction between a solute (H) and an edge dislocation if the solute is located in the slip plane, since the pressure created by the dislocation in the slip plane is zero [26]. Considering the typical stress exerting in the slip plane is shear stress, thus, H interacting with shear stresses can be assumed.

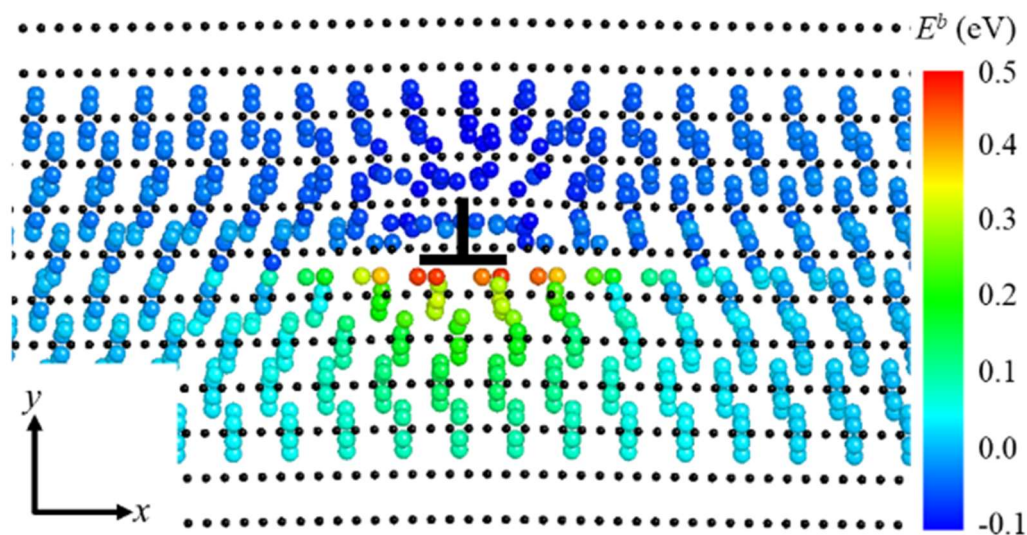


**Figure 1.** Distribution of binding energy around an edge dislocation. Small black spheres balls represent Fe atoms; large spheres represent the stable H binding sites.

More details of the distribution of H-dislocation binding energy in the slip plane can be obtained from Figure 2, where the binding energy is plotted as a function of the distance from the dislocation core. The insertion in Figure 2 shows the position of the neighboring T sites relative to the central Fe atom; from which it is seen T4–6 sites are located above the center atom, while T1–3 sites lie below it. By this definition, T5 sites lie in the slip plane; T4 sites and T6 sites are located  $\sim 0.5$  Å below the slip plane viewed along z axis. The H-dislocation binding energies at T4–6 are presented. It is very clear that the binding energies at T5 are in symmetry with respect to the core, or the binding energies at T5 are symmetrical with respect to the core ( $x = 0$ ), while the binding energies at T4 and T6 are not symmetrical to the core. It also shows that the binding energies at T6 overlap the binding energies of T5 at  $x < 0$ , while the binding energies at T6 are lower than the ones at T5 at  $x > 0$ . When the H-dislocation distance is greater than 1 nm at  $x > 0$ , the obtained binding energies are even slightly negative, indicating weak repulsive interaction between the defects. At T6 sites, the opposite features to T4 are observed. The observation of negative binding energies as well as the asymmetry distribution at T4 and T6 conflicts with the prediction of isotropic elasticity. From isotropic elasticity, the binding energy is positive on the tension side and symmetrical to the core because of the symmetric distribution of pressure generated by the dislocation.

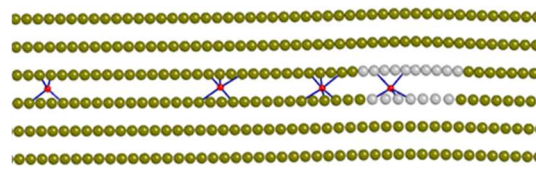
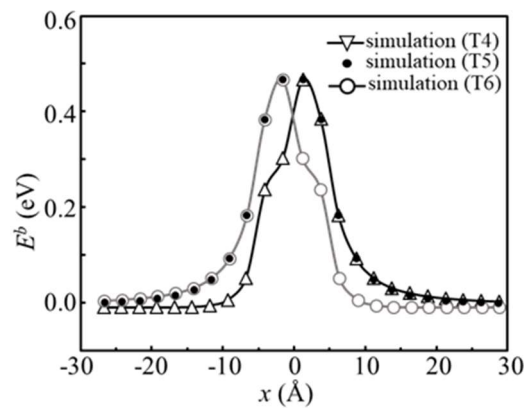


**Figure 2.** H-dislocation binding energy as a function of distance from the dislocation core with H preplaced at T4, T5 and T6 sites. The insertion displays the positions of T sites relative to the central Fe atom. The large gold spheres represent Fe atoms and the gray ones represent the neighboring T sites.

## 4. Discussion

### 4.1. H Interaction with Dislocation

When hydrogen atoms enter the strain field of other defects, they interact. The strength of the interaction is expressed by the binding energy. When the strain field of other defects is present, it will interact with them, and the strength of the interaction is expressed by the binding energy. When the strain is small,  $E_{bind}$  can be approximated by linear elasticity theory. Assume that the strain tensor caused by hydrogen at volume  $v_0$  is  $\epsilon_{ij}$ , and the stress field of the defect is  $\sigma_{ij}$ , where  $i, j = 1, 3$ , when elastic deformation occurs:

$$E^b = \sum_{i,j=1,3} v_0 \epsilon_{ij} \sigma_{ij}^d \quad (2)$$

where  $v_0$  is the volume of a Fe atom,  $\epsilon_{ij}$  is the homogeneous strains induced by H, and  $\sigma_{ij}^d$  represents the stress tensors created by the dislocation. To calculate the homogeneous strains induced by H, elastic calculation coupled with atomistic simulations are conducted. In elasticity, a point defect can be modelled as force moment tensors  $\Gamma_{ij}$  considering the defect as a point force source [36].  $\Gamma_{ij}$  can be directly calculated from atomistic simulations. Assuming a simulation box containing a point defect generates stress tensors  $\sigma_{ij}$ , the force moment tensors  $p_{ij}$  are:  $\sigma_{ij} = -\frac{1}{V} \Gamma_{ij}$ , where  $V$  is the volume of the box. Due to the symmetry of T sites in the bcc lattice, the T sites generate different force moment tensors depending on their positions relative to the central atom. Following the positions of T sites in the insertion of Figure 2, the strains of these sites in the cubic unit cell can be deduced as follows: T1 and T5 sites generate  $p_{xx} = p_{yy} \neq p_{zz}$ , T2 and T4 sites generate  $p_{zz} = p_{yy} \neq p_{xx}$  and T3 and T6 sites generate  $p_{zz} = p_{xx} \neq p_{yy}$ . For example, if H occupies a T3 site, it induces  $p_{xx} = p_{zz} = 3.7556$  eV and  $p_{yy} = 3.3586$  eV. After obtaining the force moment tensors, the H-induced strains are estimated as follows:

$$\begin{aligned} \epsilon_{11} &= \frac{1}{v_0} \frac{C_{11}p_{xx} - C_{12}p_{yy}}{(C_{11} - C_{12})(C_{11} + 2C_{12})} \\ \epsilon_{22} &= \frac{1}{v_0} \frac{-2C_{12}p_{xx} + (C_{11} + C_{12})p_{yy}}{(C_{11} - C_{12})(C_{11} + 2C_{12})} \end{aligned} \quad (3)$$

where  $C_{11} = 243.33$  GPa and  $C_{12} = 145.05$  GPa are the elastic constants used in the EAM potential. Thus, the strains of a T3 site are  $\epsilon_{11} = \epsilon_{33} = 0.112$ ,  $\epsilon_{22} = 0.056$  and obviously H creates asymmetric strains in bcc iron. When the crystal is rotated to be parallel to the dislocation orientation, the transformation of the strains is deduced by:  $\epsilon = C\epsilon C^T$ , where  $C$  is the transformation matrix which transforms the coordinates from reference state (a box with axis in  $\langle 100 \rangle$  directions) into new state (a box with axis parallel to the dislocation orientation) and  $C^T$  is the transpose of  $C$ . The strains at various T sites thus are computed.

If one only considers the dilatation of H interstitials, i.e., all components of  $\epsilon_{ij}$  are equal, the interaction reduces to:

$$E^b = -p\Delta V \quad (4)$$

where  $p = -1/3 \sum_i \sigma_{ii}$  is the pressure created by the dislocation and  $\Delta V$  is the volume expansion of H in Fe. The value of  $\Delta V$  is  $3.26 \text{ \AA}^3$  calculated from the corresponding dipole tensor following the method of Schober and Ingle.

When studying H-dislocation interactions, one can use either anisotropic elasticity or isotropic elasticity to describe the stress tensors created by the dislocation [26,37]. For anisotropic calculations the elastic constants given by the EAM potential are used:  $C_{11} = 243.33$  GPa,  $C_{12} = 145.05$  GPa and  $C_{44} = 116.15$  GPa. For isotropic elasticity, the equivalent elastic constants are needed. In our study, the shear modulus  $\mu$  and Poisson's ratio  $\nu$  are obtained by the Voigt average of elastic constants given by the potential, which are  $\mu = 89.3$  GPa and  $\nu = 0.285$ , respectively.

#### 4.2. Comparison with Atomistic Simulations

A comparison of the H-dislocation binding energies between atomistic simulations and isotropic elasticity are presented in Figure 3. Two types of calculations are performed using elasticity to study H-dislocation interactions: calculations only considering dilation and calculations considering all strains induced by H. In these calculations, it is assumed that H-induced strains in the strained crystal are the same as the ones generated at T sites in the perfect crystal. Considering the strains of the crystal induced by a dislocation is small except the core region, this assumption is reasonable. When H is pre-placed at T5 sites (Figure 3a), perfect agreement between elasticity and simulations is observed at the H-dislocation distance greater than  $\sim 19 \text{ \AA}$ , and within this distance elasticity underestimates the binding energies. Since elasticity predicts zero pressure precisely in the slip plane, if one only considers the dilation effect of H placed close to the slip plane, there are weak interactions between H and the dislocation. Moreover, the two calculations predict almost the same binding energies. This is because H at T5 sites only generates strains along the axis but no shear components, and the calculations using Equations (2) and (4) are identical. However, when H is placed at T4 sites, which generates a shear component  $\epsilon_{12} = 2.27\%$ , the situation changes. Based on Figure 4b, it is clear that, if considering all strains induced by H, the obtained binding energies agree better with simulations than those considering only dilation. Thus, shear strains are attributed to H-dislocation interactions. It is noted that the shear stress created by the edge dislocation at  $x < 0$  is negative, because the product of  $\sigma_{12}^d \epsilon_{12}$  is negative at  $x < 0$  (i.e., repulsive H-dislocation interactions), while the  $\sigma_{12}^d \epsilon_{12}$  is positive at  $x > 0$ , (i.e., attractive H-dislocation interactions). Therefore, the H-dislocation binding energies are lower at  $x < 0$  than the ones at  $x > 0$  at T4 sites, as presented in Figure 2. Because T6 sites and T4 sites generate the same axial strains, but the opposite and equivalent shear strains, the results at T6 sites are the reflection of the ones at T4 sites with respect to  $x = 0$  (Figure 2).

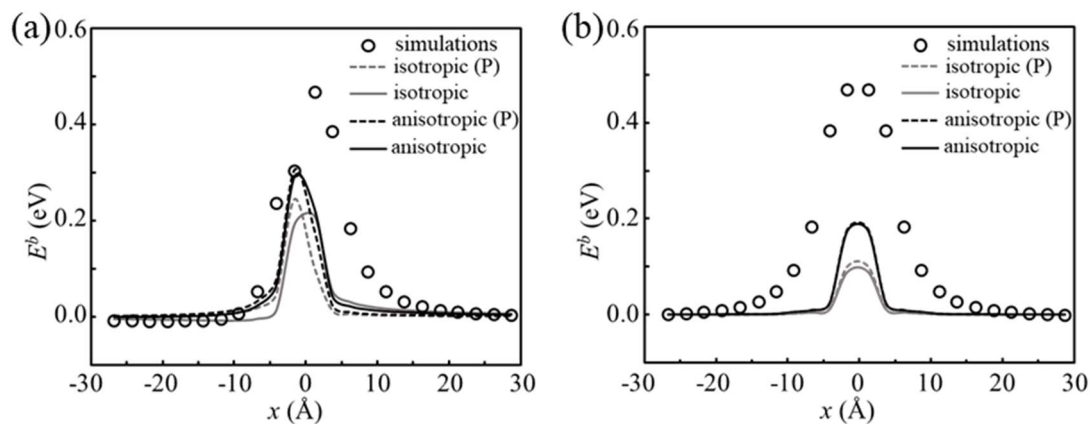


**Figure 3.** Binding energies between a H atom and an edge dislocation for different  $x$  positions with H pre-placed at T5 sites (a) and T4 sites (b) in the slip plane. The elasticity considers only dilation or all strain components induced by H, using isotropic elasticity or anisotropic elasticity.

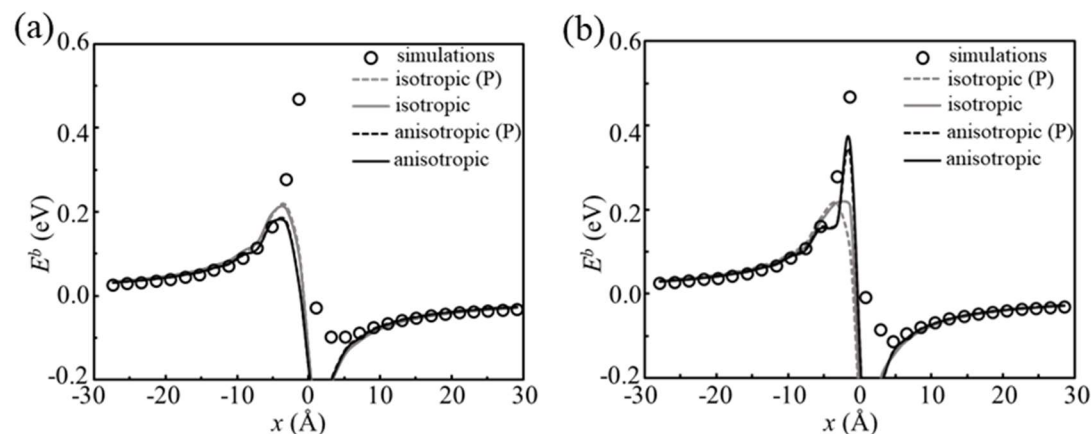


**Figure 4.** Binding energies between a H atom and an edge dislocation for different  $y$  positions with H pre-placed at T5 sites (a) and T4 sites (b), along the  $y$  axis. The elasticity considers only dilation or all strain components induced by H, using isotropic elasticity or anisotropic elasticity.

When the dislocation stresses are represented using anisotropic elasticity, the validity of elasticity is at H-dislocation distance larger than  $\sim 19$  Å, i.e., the same as the isotropic predictions. However, the two types of calculations predict almost the same binding energies at both T5 sites and T4 sites (Figure 3b). Since anisotropic elasticity predicts binding energies including multiple shear strains ( $\epsilon_{12}$ ,  $\epsilon_{13}$  and  $\epsilon_{23}$ ) effect, while isotropic elasticity only contains contribution of  $\epsilon_{12}$ , the binding energies using anisotropic elasticity are the collective effect of all these strain components and may lead to equivalent results to those only considering dilation.

A comparison of the binding energies in the  $\langle -110 \rangle$  direction is made in Figure 4, where the  $x$  component of interstitial sites to the core is about 1.5 Å and the  $y$  component varies. It is clear elasticities agree fairly well with simulations considering only dilation or all stress components, using isotropic elasticity or anisotropic elasticity. The valid range of elasticity is greater than 5 Å from the core. This cutoff distance is very close to the core radius  $\sim 2b$  usually applied in other studies.

#### 4.3. Influences of Octahedral Sites

Instead of assuming H occupying T sites when stable, one can assume that H occupies an octahedral site (O site). In fact, O sites can have stronger H trap-energy than T sites in bcc iron under pure shear strains, depending on the position of H relative to the central Fe [38,39]. Anisotropic strains in bcc iron can induce a solution energy at an O site as low

as that at T site, resulting in enhancement of H atmosphere. Considering the complicated stress fields around a dislocation and the short distance between a T site and a neighboring O site ( $\sim 0.71$  Å), H may easily migrate to neighboring O sites from initial T sites. There are two nearest O sites in the neighborhood of a T site; the relative positions of the T sites and O sites are represented in Figure 5a,b. A comparison of the simulation results and elasticity assuming H at T5 sites or O2 sites or O6 sites is displayed in Figure 6. It is seen that the elastic calculations assuming hydrogen at O sites agree better with simulations near the core than that at T sites, while the calculations at T sites precisely agree with simulations far away from the core.

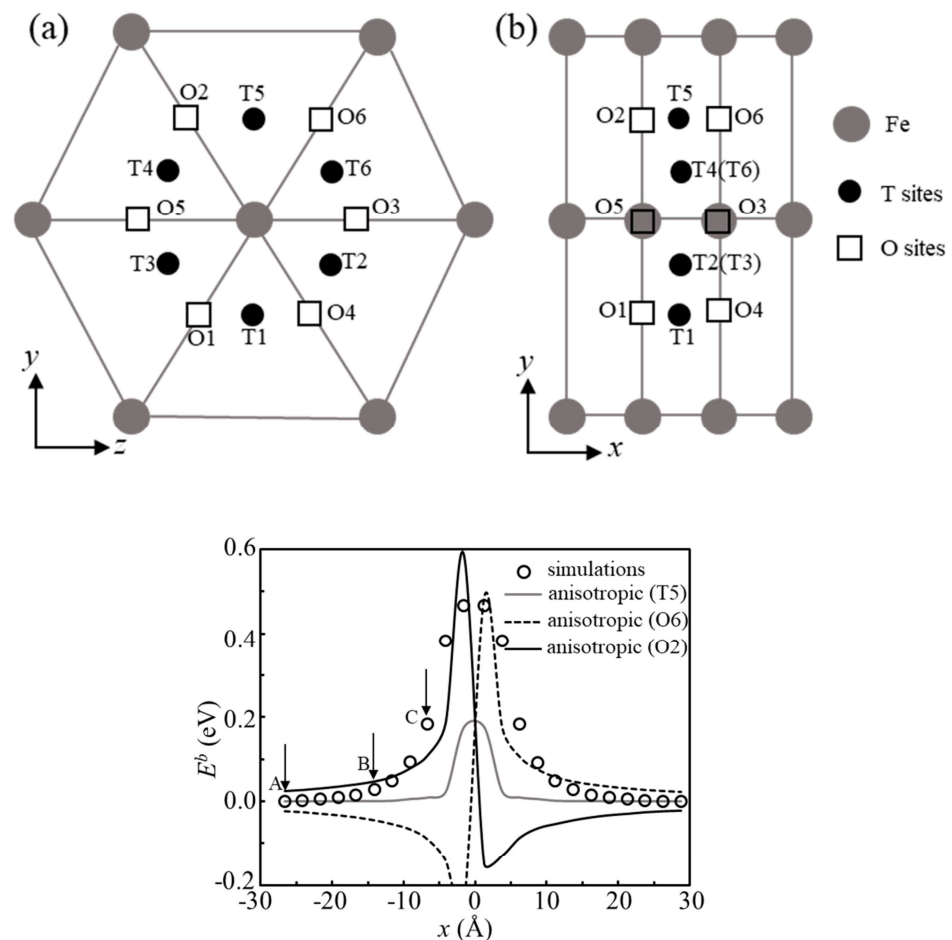


**Figure 5.** Binding energies between a H atom and an edge dislocation for different  $x$  positions assuming H at T5 sites or O2 sites or O6 sites. The stresses of the dislocation are represented using isotropic and anisotropic elasticity. (a) the two O sites closest point to T, (b) the relative positions of the T sites and O sites.

The results can be roughly divided into three stages:

1. The first stage where  $|x| > 19$  Å, and elasticity assuming H at T5 sites accurately describes the binding energy, while O sites overestimate (O6) or underestimate (O2) the energies;
2. The second stage ( $9$  Å  $< |x| < 19$  Å), where atomistic results are in the middle of the results at T5 sites and at O6 sites ( $x < 0$ ) or O2 sites ( $x > 0$ );
3. The third stage ( $|x| < 9$  Å), where elastic calculations underestimate the binding energies.

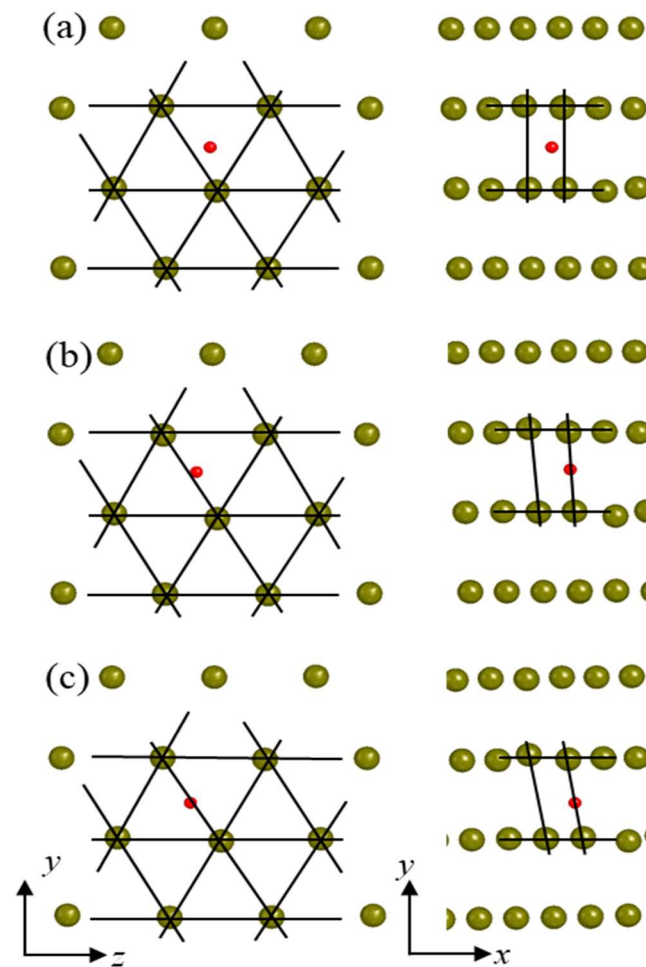


**Figure 6.** Equilibrium configurations show the relative H positions in different stages. (a–c) represent the configurations of point A, B and C in Figure 5, respectively. Projection on the  $x$  plane is displayed on the left and projection on the  $z$  plane is on the right. The gold spheres represent Fe atoms and the red spheres represent H atoms.

The equilibrium configurations of H-dislocation interactions are presented in Figure 6 to observe the position of a H atom relative to the central Fe. The configurations correspond to the labels in Figure 6, and represent H-dislocation structures in the three stages mentioned above. The observation is performed along both  $x$  axis and  $z$  axis and the results are presented in Figure 6 on the left (along  $x$  axis) and right (along  $z$  axis). In Figure 6a, H is located in the upper triangle and towards the edge viewed from  $x$  direction; projection in the  $z$  plane shows H placed between two Fe arrays and closer to the right array. Therefore, H occupies a T5 site at point A. H lies just beside the midpoint of two Fe arrays in Figure 6b, while precisely at the middle point in Figure 6c when viewed in the  $x$  direction. When viewed from the  $z$  direction, H is located at the midpoint of Fe arrays in the neighboring planes. A comparison of H positions in Figure 6 and the sites in Figure 1 reveals that H prefers to occupy an O2 site at point C and a site closer to O2 at point B.

The H-dislocation interaction further from the core is intrinsically the product of strains induced by H and stress tensors generated by the dislocation. In the slip plane, the contribution from axial stresses is negligible (weak axial stresses), and the dominant interactions are shear strains with shear tensors [40]. From the point of view of energy, H prefers to occupy an octahedral site rather than a tetrahedral site to lower the total energy of the system, since at an octahedral site H induces  $\sim 0.2$  shear strain ( $\epsilon_{xy}$ ), eight times that induced at a tetrahedral site. A large number of hydrogen atoms can be trapped in the slip

plane forming a wide area of H atmosphere around the dislocation, which exerts a strong drag effect for slipping dislocations [14,41].

## 5. Conclusions

The interaction between H and an edge dislocation in bcc iron is investigated using EAM potential for a H-Fe system. The sites with strong binding energy are found at the dislocation core, as well as in the slip plane, suggesting high H concentration can form along the slip plane. The interstitial H not only interacts with hydrostatic stress, but also with the shear stresses generated by the dislocation, in particular the slip plane.

The atomistic simulations are then used to check the applicability of elastic theory. When the separation distance between H and dislocation is greater than 19 Å, elasticity quantitatively predicts H-dislocation interaction. One can use isotropic or anisotropic elasticity to describe this interaction, since the predictions made by them only generate slight differences. When H lies closer to the dislocation, good agreement with simulations is obtained if considering all strains induced by H at the octahedral sites and using anisotropic elasticity.

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**Conflicts of Interest:** The authors declare no conflict of interest.

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